Claims

1-4. (canceled)

5. (previously presented) A computer-implemented method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure, wherein the identifying includes tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and, when an unacceptable state is detected, backtracking the path to the last assignment that was made;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation one or more candidates based on the evaluation;

producing fixed bond information based on the selection; and

outputting the produced fixed bond information.

6. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. (canceled).

8. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes an acyclic system.

9. (previously presented). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure, wherein the identifying includes

tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and backtracking the path to the last selection that was made, when an unacceptable state is detected;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation one or more candidates based on the evaluation;

producing fixed bond information based on the selection;

based on the fixed bond information, producing a fixed bond representation that includes a pair of opposite charges lacked by the delocalized representation; and

outputting the produced fixed bond representation.

10. (previously presented). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure, wherein the identifying includes tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and backtracking the path to the last selection that was made, when an unacceptable state is detected;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection;

based on the fixed bond information, producing a fixed bond representation that includes a pair of radicals lacked by the delocalized representation; and

outputting the produced fixed bond representation.

11. (previously presented). The method of claim 5, wherein the assigning atomic charges or radicals is performed based on electronic state and valence distribution (ESVD), and further comprising:

queuing at least a subset of the ESVDs by priority.

12. (previously presented). A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure, wherein the identifying includes tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and backtracking the path to the last selection that was made, when an unacceptable state is detected;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation;

producing fixed bond information based on the selection;

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation; and

outputting the produced fixed bond information.

13. (previously presented). The method of claim 12, wherein the table is configured to allow additional elements and values to be added.

14. (previously presented). The method of claim 12, wherein the table is configured to allow additional elements and values to be added to apply to any chemical element.

15. (previously presented). The method of claim 5, further comprising:

deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. (previously presented). The method of claim 5, further comprising:

determining, by either exhaustion or exceeding a predetermined amount of time, whether it is possible to produce a neutral, non-radical fixed bond representation of most chemical structures.

17 and 18. (canceled).

19. (previously presented). The method of claim 5, wherein at least a portion of the delocalized representation describes a monocyclic ring system.

20. (currently amended). A computer-implemented system for ~~use in~~ deriving fixed bond information, comprising:

an analyzer ~~analyzing~~ configured to analyze a delocalized representation of a chemical structure, wherein at least a portion of the delocalized representation describes a polycyclic ring system;

an identifier ~~identifying~~ configured to identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator ~~evaluating~~ configured to evaluate at least a subset of the fixed bond representation candidates;

a selector ~~electing~~ configured to elect from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer ~~producing~~ configured to produce fixed bond information based on the selection;

said produced fixed bond information being output by the system.

21. (previously presented). Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a delocalized representation of a chemical structure, wherein at least a portion of the delocalized representation describes a polycyclic ring system;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure, wherein the identifying includes

tracing a path through the structure, assigning bond orders and atomic charges or radicals as the path is traced, and backtracking the path to the last selection that was made, when an unacceptable state is detected;

evaluate at least a subset of the fixed bond representation candidates;

select from among the plurality of fixed bond representation candidates based on the evaluation;

produce fixed bond information based on the selection; and

outputting the produced fixed bond information.

22. (canceled).

23. (canceled).

24. (canceled).

25. (canceled).

26. (canceled).

27. (canceled).

28. (previously presented) The method of claim 5, wherein when the evaluating determines that a fixed bond representation candidate cannot be improved upon, it is selected.

29. (previously presented) The method of claim 11, wherein the highest priority ESVD is assigned and the remainder of the at least a subset of the ESVDs are placed in an independent queue.